

On the number of contacts of a floating polymer chain crosslinked with a surface adsorbed chain on fractal structures

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Abstract. We study the interaction problem of a linear polymer chain, floating in fractal containers that belong to the three-dimensional Sierpinski gasket (3D SG) family of fractals, with a surface-adsorbed linear polymer chain. Each member of the 3D SG fractal family has a fractal impenetrable 2D adsorbing surface, which appears to be 2D SG fractal. The two-polymer system is modelled by two mutually crossing self-avoiding walks. By applying the Monte Carlo Renormalization Group (MCRG) method, we calculate the critical exponents φ , associated with the number of contacts of the 3D SG floating polymer chain, and the 2D SG adsorbed polymer chain, for a sequence of SG fractals with $2 \leq b \leq 40$. Besides, we propose the codimension additivity (CA) argument formula for φ , and compare its predictions with our reliable set of the MCRG data. We find that φ monotonically decreases with increasing b , that is, with increase of the container fractal dimension. Finally, we discuss the relations between different contact exponents, and analyze their possible behaviour in the fractal-to-Euclidean crossover region $b \rightarrow \infty$.

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1. Introduction

The self-avoiding walk (SAW) is a random walk that must not contain self-intersections. This kind of random walk, placed on a lattice, has been widely used as a model of a linear polymer in a good solvent [1]. Even though an isolated polymer chain is difficult to observe experimentally, numerous studies of the single-chain statistics have been upheld as a requisite step towards understanding the statistics of collection-chain systems [2]. A reasonable extension of a single polymer concept is a model of two interacting linear polymers (two interacting SAWs), which has been a subject of extensive studies because of its theoretical and practical interest. To investigate the critical properties of the two-chain (or many-chain) systems various theoretical techniques have been applied, including the field theoretical approach [3], Monte Carlo simulations [4, 5], transfer-matrix calculations [6], and renormalization group (RG) methods [7–9]. Among other fields, a system of two interacting SAWs, that are mutually avoiding, has been successfully applied as a model of diblock copolymers [10, 11], as well as in the studies of double-stranded DNA molecules [12–14].

In order to study the number of contacts between monomers that belong to different polymers, the two-polymer system may be modelled by two mutually crossing self-avoiding walks [15, 16], that is, by two SAWs whose paths on an underlying lattice can cross (intersect) each other. Each crossing between two SAW paths corresponds to a contact of two monomers that belong to different polymer chains, and therefore with each crossing we may associate the contact energy ϵ_c . In analogy with the problem of polymer adsorption onto a hyperplane [17], we may assume that with decreasing of temperature the number of crossings M increases so that at the critical temperature T_c it behaves according to the power law

$$M \sim N^\varphi, \quad (1)$$

where N is the total number of monomers in the longer chain, and φ is the crossover critical exponent. Below T_c the number of contacts becomes proportional to N , whereas above T_c it is vanishingly small.

In spite of different approaches to the two-SAW problem, the entire physical picture achieved so far, is almost entirely of a phenomenological character and there are only few numerical results. For instance, in the case of Euclidean lattices, besides the codimension additivity (CA) argument predictions for the contact critical exponents (with conjectures $\varphi = 1/2$ in $d = 2$, and $\varphi \approx 1/5$ in $d = 3$), there is only Monte Carlo result $\varphi = 0.516 \pm 0.005$, for a model of two mutually crossing SAWs on the square lattice [16]. The above problem has been also studied on fractal lattices. But, in the case of fractals it may be noted that the two-dimensional (2D) fractal lattices (embedded in the 2D Euclidean space) have been more frequently investigated [15, 18, 19] than the corresponding model in the case of 3D fractal structures [20]. Since the 3D fractals definitely may serve as a better description of real systems (porous media, for instance), it is recommendable to study the described model in a case of a set of 3D fractals. For

this reason, it is desirable to extend the study of two-polymer system on a family of fractal lattices whose characteristics approach properties of a 3D Euclidean lattice.

In this paper we report results of our study for the contact critical exponent φ of two polymer chains, that display inter-chain interactions, in the three-dimensional fractal lattices that belong to the Sierpinski gasket (SG) family of fractals. The two-polymer system is modelled by two SAWs which are allowed to cross each other. We assume that the first polymer is a floating chain in the bulk of 3D SG fractal, while the second polymer chain is adsorbed onto one of the four surfaces (which is, in fact, 2D SG fractal) by which is 3D SG fractal bounded. In section 2 of the paper, we first describe the 3D SG fractals for general b . Then, we present the framework of the RG method for studying statistics of two mutually crossing SAW chains, taking into account the presence of the inter-chain interactions, in a way that should make the method transparent for the Monte Carlo calculations of the contact critical exponent φ . In section 3 we present the obtained specific values of φ for a sequence of 3D SG fractals, that is, for $2 \leq b \leq 40$. In the same section we propose the phenomenological formulae for φ , based on the CA arguments, test their predictions on the obtained MCRG data, and discuss relations between different contact exponents. Summary of the obtained results and the relevant conclusions are given in section 4.

2. Monte Carlo renormalization group approach

In this section we are going to apply the Monte Carlo renormalization group (MCRG) method to the studied model of interacting polymers on the 3D SG family of fractals. These fractals have been studied in numerous papers so far, and consequently we shall give here only a requisite brief account of their basic properties. It starts with recalling the fact that each member of the 3D SG fractal family is labelled by an integer $b \geq 2$ and can be constructed in stages. At the first stage ($r = 1$) of the construction there is a tetrahedron of base b that contains $b(b+1)(b+2)/6$ upward oriented unit tetrahedrons. The subsequent fractal stages are constructed recursively, so that the complete self-similar fractal lattice can be obtained as the result of an infinite iterative process of successive ($r \rightarrow r+1$) enlarging the fractal structure b times, and replacing the smallest parts of enlarged structure with the initial structure $r = 1$ (see for instance, figure 1 of [21]). Fractal dimension d_f of the 3D SG fractal is equal to

$$d_f^{3D} = \ln[b(b+1)(b+2)/6] / \ln b. \quad (2)$$

We assume here that one of the four boundaries of the 3D SG fractal is an impenetrable adsorbing surface, which is itself a 2D SG fractal with the fractal dimension

$$d_f^{2D} = \ln[b(b+1)/2] / \ln b. \quad (3)$$

In the terminology that applies to the SAW, we assign the weight x_3 to a step of the SAW in the bulk (3D SG fractal), which represents a floating polymer (we mark it by P_3), and the weight x_2 to a step of the SAW adsorbed on the surface (2D SG fractal), which represents an adsorbed polymer (marked by P_2), whose monomers act

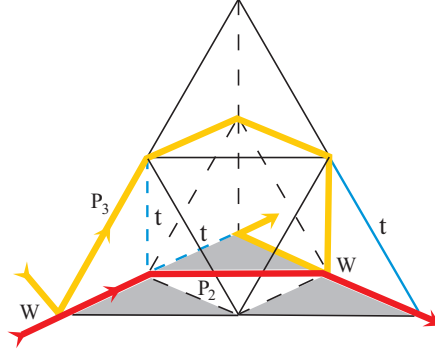


Figure 1. The structure of the three-dimensional SG fractal, for $b = 2$, at the first stage of construction, with an example of the bulk polymer chain (P_3) depicted by yellow line and the surface-adsorbed polymer chain (P_2) depicted by red line. The shaded area represents the adsorbing surface (the two-dimensional SG fractal). The two polymers are crosslinked at the two sites, so that each contact contributes the weight factors w . The blue bonds, marked by t , describe the interactions between those monomers which are nearest neighbors to the crosslinked points. Thus, the depicted two-polymer configuration contributes the weight $x_3^5 x_2^3 w^2 t^3$ in the corresponding RG equation (especially, in the equation (7) for $i = 2$ and $r = 0$).

as pinning sites for the floating polymer. In order to explore interacting effects of two SAWs on the underlying fractals, we introduce the two Boltzmann factors $w = e^{-\epsilon_c/k_B T}$ and $t = e^{-\epsilon_t/k_B T}$, where ϵ_c is the energy of two monomers in contact (which occurs at a crossing site of SAWs), while ϵ_t is the energy associated with two sites which are nearest neighbours to a crosslinked site and which are visited by different SAWs (see figure 1).

To describe all possible configurations of the two-chain polymer system, within the accepted model, we need to introduce the nine restricted partition functions $A^{(r)}$, $B^{(r)}$, $C^{(r)}$, $A_i^{(r)}$ ($i = 1, 2, 3, 4$), and $B_i^{(r)}$ ($i = 1, 2$), that are depicted in figure 2. The recursive nature of the fractal construction implies the following recursion relations for restricted partition functions

$$A^{(r+1)} = \sum_{N_A, N_B} a(N_A, N_B) A^{N_A} B^{N_B}, \quad (4)$$

$$B^{(r+1)} = \sum_{N_A, N_B} b(N_A, N_B) A^{N_A} B^{N_B}, \quad (5)$$

$$C^{(r+1)} = \sum_{N_C} c(N_C) C^{N_C}, \quad (6)$$

$$A_i^{(r+1)} = \sum_{\mathcal{N}} a_i(\mathcal{N}) A^{N_A} B^{N_B} C^{N_C} \prod_{j=1}^4 A_j^{N_{A_j}} \prod_{k=1}^2 B_k^{N_{B_k}}, \quad i = 1, 2, 3, 4, \quad (7)$$

$$B_i^{(r+1)} = \sum_{\mathcal{N}} b_i(\mathcal{N}) A^{N_A} B^{N_B} C^{N_C} \prod_{j=1}^4 A_j^{N_{A_j}} \prod_{k=1}^2 B_k^{N_{B_k}}, \quad i = 1, 2, \quad (8)$$

where \mathcal{N} denotes the set of numbers $\mathcal{N} = \{N_A, N_B, N_C, N_{A_1}, N_{A_2}, N_{A_3}, N_{A_4}, N_{B_1}, N_{B_2}\}$, and, where we have omitted the superscript (r) on the right-hand side of the above relations. The self-similarity of the fractals implies that the sets of coefficients a, b

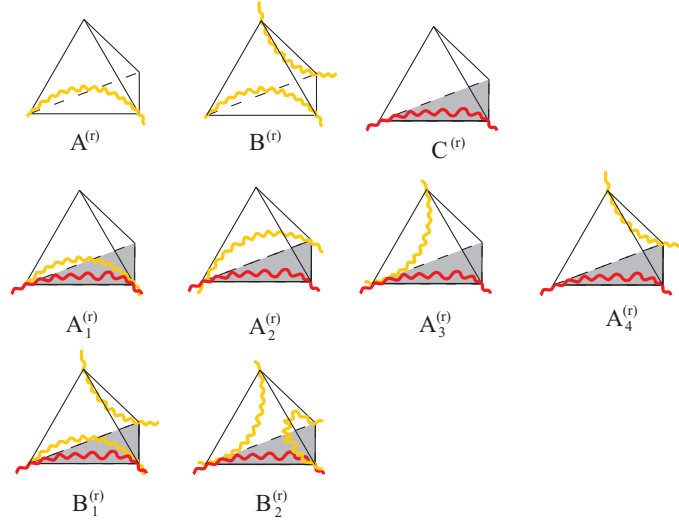


Figure 2. Schematic representation of the nine restricted generating functions used in the description of all possible two-SAW configurations, within the r -th stage of the 3D SG fractal structure. Thus, for example, the $A_1^{(r)}$ represents the configuration when both polymers (3D SG floating and 2D SG adsorbed) pass through the same vertices of a particular r -th stage of the fractal lattice. The interior details of the r -th stage fractal structure, as well as details of the chains, are not shown (for the chains, they are manifested by the wiggles of the SAW paths).

and c , that describe a single polymer configurations (a and b coefficients describe the bulk polymer configurations, whereas the c coefficients describe the adsorbed polymer configurations), and the sets of coefficients a_i and b_i of the corresponding two-chain configurations do not depend on r . Each of the two-chain coefficients (a_i and b_i) represents the number of ways in which the corresponding parts of the two-SAW configuration, within the $(r + 1)$ -th stage fractal structure, can be comprised of the two-SAW configurations within the fractal structures of the next lower order. Because of the independence of r , these coefficients can be calculated by studying all two-SAW paths within the fractal generator only, that is on the first step of construction $r = 1$.

The above set of relations (4)–(8), can be considered as the RG equations for the problem under study, with the initial conditions: $A^{(0)} = x_3$, $B^{(0)} = x_3^2$, $C^{(0)} = x_2$, $A_1^{(0)} = x_3x_2w^2$, $A_2^{(0)} = A_3^{(0)} = x_3x_2wt$, $A_4^{(0)} = x_3x_2$ and $B_1^{(0)} = B_2^{(0)} = x_3^2x_2w^2$, which correspond to the unit tetrahedron. On the physical grounds that are reasonable for the studied model [22], one can expect that the RG transformations should have three relevant fixed points of the general type

$$(A^*, B^*, C^*, A_1^*, A_2^*, A_3^*, A_4^*, B_1^*, B_2^*). \quad (9)$$

The first fixed point

$$(A^*, B^*, C^*, 0, 0, 0, A_4^*, 0, 0), \quad (10)$$

with $A_i^* = 0$ ($i = 1, 2, 3$), $A_4^* = A_4^*(A^*, B^*, C^*)$ and $B_i^* = 0$ ($i = 1, 2$), due to the meaning of these quantities (see figure 2), describes segregated phase of two chain polymers that

should be expected in the high temperature region $T > T_c$. The second fixed point

$$(A^*, B^*, C^*, A^*C^*, A^*C^*, A^*C^*, A^*C^*, B^*C^*, B^*C^*), \quad (11)$$

with $A_i^* = A^*C^*$ ($i = 1, 2, 3, 4$) and $B_i^* = B^*C^*$ ($i = 1, 2$), which appears to be a tricritical point, describes the state of the two-polymer system that occurs at the critical temperature $T = T_c$ when segregated and entangled polymer phases become identical. Finally, the third fixed point

$$(0, 0, 0, C^*, 0, 0, 0, 0, 0), \quad (12)$$

with the nonzero value only for $A_1^* = C^*$, describes the polymer entangled state, which should appear at low temperatures $T < T_c$.

In what follows we focus our attention on the tricritical fixed point (11) to calculate the contact critical exponent φ_{32} between P_3 and P_2 polymer chains. We can observe that the above system of RG equations (4)–(8) can be split into three uncoupled sets of RG equations: (4)–(5), (6), and (7)–(8). Moreover, it should be noticed, that for each b , the first two sets of RG equations, (4)–(5) and (6), have only one nontrivial fixed point value (A^*, B^*) [21] and C^* [23] respectively, which thereby completely determine the coordinates of the tricritical fixed point. Calculation of φ_{32} starts with solving the eigenvalue problem of the RG equations (4)–(8), linearized at the tricritical fixed point. The related eigenvalue problem can be separated into three parts. The first part of the eigenvalue problem, related to the equations (4)–(5) gives the eigenvalue λ_{ν_3} of the end-to-end distance critical exponent $\nu_3 = \ln b / \ln \lambda_{\nu_3}$ of the 3D SG floating polymer, while the second part, related to the equation (6), gives the eigenvalue λ_{ν_2} of the end-to-end distance critical exponent $\nu_2 = \ln b / \ln \lambda_{\nu_2}$ of the 2D SG SAW, that represents the adsorbed polymer. Finally, the third part of the eigenvalue problem (related to the equations (7)–(8)) reduces to solving the equation

$$\det \left| \left(\frac{\partial X'_i}{\partial X_j} \right)^* - \lambda \delta_{ij} \right| = 0, \quad (13)$$

where X_i are elements of the set $\{A_1, A_2, A_3, A_4, B_1, B_2\}$, and the asterisk means that the derivatives should be taken at the tricritical fixed point. Also, we have used the prime symbol as a superscript for the $(r + 1)$ -th restricted partition functions and no indices for the r -th order partition functions. The largest eigenvalue $\lambda_{\varphi_{32}}$ of above equation determines the contact critical exponent via the formula

$$\varphi_{32} = \frac{\ln \lambda_{\varphi_{32}}}{\ln \lambda_{\nu_3}}. \quad (14)$$

Hence, in an exact RG evaluation of φ_{32} one needs to calculate partial derivatives of sums (4)–(8), and thereby one should find the coefficients a, b, c, a_i , and b_i . The latter can be calculated by an exact enumeration of all possible two-SAW configurations for each particular b . We have found that this enumeration is feasible only for small b . However, for large b the exact enumeration turns out to be a forbidding task. We bypass this problem by applying the MCRG method. Within this method, the first step would be to locate the tricritical fixed point. To this end, we may observe that the

results obtained in [21] provide information for both (A^*, B^*) and λ_{ν_3} for a sequence of 3D SG fractals with $2 \leq b \leq 40$, whereas the results obtained in [24] give the fixed point values of C^* for 2D SG fractals, for b in the range $2 \leq b \leq 80$. Accordingly, the next step in the MCRG method consists of finding $\lambda_{\varphi_{32}}$ without explicit calculation of the RG equation coefficients.

To solve the partial eigenvalue problem (13), so as to learn $\lambda_{\varphi_{32}}$, we need to find the requisite 36 partial derivatives. These derivatives can be related to various averages of the numbers N_{A_i} and N_{B_i} of different crossings of the SAWs for various two-SAW configurations that correspond to the restricted partition functions $A_i^{(r)}$ and $B_i^{(r)}$. For instance, starting with (7) (in the notation that does not use the superscripts $(r+1)$ and r) and by differentiating it with respect to A_1 we get

$$\frac{\partial A'_i}{\partial A_1} = \sum_{\mathcal{N}} N_{A_1} a_i(\mathcal{N}) A^{N_A} B^{N_B} C^{N_C} A_1^{-1} \prod_{j=1}^4 A_j^{N_{A_j}} \prod_{k=1}^2 B_k^{N_{B_k}}, \quad i = 1, 2, 3, 4. \quad (15)$$

Now, assuming that A'_i represents the grand canonical partition functions for the ensemble of all possible two-SAW configurations, where each of two SAWs starts and leaves fractal generator at two fixed corners, so that the first SAW is a 3D SG floating chain, while the other SAW is a 2D SG adsorbed chain. With this concept in mind, we can write the corresponding ensemble average

$$\langle N_{A_1} \rangle_{A'_i} = \frac{1}{A'_i} \sum_{\mathcal{N}} N_{A_1} a_i(\mathcal{N}) A^{N_A} B^{N_B} C^{N_C} \prod_{j=1}^4 A_j^{N_{A_j}} \prod_{k=1}^2 B_k^{N_{B_k}}, \quad i = 1, 2, 3, 4, \quad (16)$$

which can be directly measured in a Monte Carlo simulation. Combing (15) and (16) we can express the requisite partial derivative in terms of the measurable quantity

$$\frac{\partial A'_i}{\partial A_1} = \frac{A'_i}{A_1} \langle N_{A_1} \rangle_{A'_i}, \quad i = 1, 2, 3, 4. \quad (17)$$

In a similar way we can find the rest derivatives, so that all needed derivatives, calculated in the tricritical fixed point, may be related with the corresponding averages

$$\left(\frac{\partial A'_i}{\partial A_j} \right)^* = \langle N_{A_j} \rangle_{A'_i}^*, \quad \left(\frac{\partial A'_i}{\partial B_k} \right)^* = \frac{A^*}{B^*} \langle N_{B_k} \rangle_{A'_i}^*, \quad i, j = 1, 2, 3, 4; \quad k = 1, 2, \quad (18)$$

$$\left(\frac{\partial B'_l}{\partial A_j} \right)^* = \frac{B^*}{A^*} \langle N_{A_j} \rangle_{B'_l}^*, \quad \left(\frac{\partial B'_l}{\partial B_k} \right)^* = \langle N_{B_k} \rangle_{B'_l}^*, \quad j = 1, 2, 3, 4; \quad k, l = 1, 2. \quad (19)$$

Consequently to solve the eigenvalue problem (13), so as to learn $\lambda_{\varphi_{32}}$, we need to find the above partial derivatives at the tricritical fixed point. These derivatives are related to various averages of the numbers N_{A_j} , and N_{B_k} , of different two-SAW parts (of the types A_j , and B_k) within the corresponding two-SAW configurations (described with A'_i or B'_l). Therefore, to calculate the derivatives (18)–(19) at the tricritical fixed point, one needs 36 averages ($\langle N_{A_j} \rangle_{A'_i}^*$, $\langle N_{B_k} \rangle_{A'_i}^*$, $\langle N_{A_j} \rangle_{B'_l}^*$, $\langle N_{B_k} \rangle_{B'_l}^*$), which are all measurable through Monte Carlo simulations. The pertinent Monte Carlo technique has been described in [24], and we would not like to elaborate on them here. Solving numerically the eigenvalue equation (13) we obtain $\lambda_{\varphi_{32}}$, and, finally, using relation (14), we calculate the contact critical exponent φ_{32} , whose specific values we present in the next section.

Table 1. The MCRG ($2 \leq b \leq 40$) results obtained in this work for the contact critical exponents φ_{32} for the 3D SG family of fractals. For the completeness we quote here the MCRG values for the RG parameters (A^* , B^*) [21], and C^* [24].

b	A^*	B^*	C^*	φ_{32}
2	0.4311±0.0009	0.0505±0.0023	0.61825±0.00061	0.5440±0.0056
3	0.3421±0.0004	0.0245±0.0015	0.55137±0.00044	0.4969±0.0024
4	0.2898±0.0004	0.0122±0.0020	0.50658±0.00034	0.4658±0.0006
5	0.2560±0.0004	0.0067±0.0019	0.47455±0.00028	0.4451±0.0012
6	0.2319±0.0003	0.0038±0.0012	0.45091±0.00024	0.4250±0.0004
7	0.2148±0.0003	0.0020±0.0018	0.43240±0.00021	0.4092±0.0008
8	0.2016±0.0003	0.0012±0.0026	0.41780±0.00019	0.3963±0.0006
9	0.1912±0.0004	0.0007±0.0008	0.40574±0.00017	0.3841±0.0007
10	0.1829±0.0003	0.0005±0.0023	0.39586±0.00007	0.3714±0.0005
12	0.1703±0.0004	0.0001±0.0035	0.38037±0.00013	0.3514±0.0004
15	0.1581±0.0001	–	0.36396±0.00011	0.3226±0.0003
17	0.1526±0.0001	–	0.35593±0.00008	0.3126±0.0003
20	0.1462±0.0001	–	0.34681±0.00006	0.2956±0.0003
25	0.1399±0.0001	–	0.33602±0.00008	0.2677±0.0003
30	0.1353±0.0001	–	0.32876±0.00007	0.2573±0.0002
35	0.1327±0.0001	–	0.32350±0.00008	0.2183±0.0003
40	0.1305±0.0001	–	0.31936±0.00006	0.2016±0.0003

3. Results and discussion

We have studied the interaction problem of a floating polymer chain confined in the 3D SG fractal container, with a surface (2D SG fractal) adsorbed polymer chain to calculate the critical exponent φ_{32} which governs the number of contacts between two chains.

The main goal of this study is the MCRG evaluation of φ_{32} , for various values of b . Furthermore, in the case $b = 2$, we have calculated the exact value. To find the exact forms of RG equations (4)–(8), for $b = 2$ fractal, using the computer facilities we have been able to enumerate all coefficients (which are available upon request addressed to the author) that appear in these equations. Linearization of obtained RG equations around the tricritical fixed point (11), in this case determined by the values $A^* = 0.4294$, $B^* = 0.0499$ and $C^* = 0.6180$ [25], gives the following eigenvalues: $\lambda_{\nu_3}(b = 2) = 2.7965$ and $\lambda_{\varphi_{32}}(b = 2) = 1.7475$, whereupon we find the exact value $\varphi_{32}(b = 2) = \ln 1.7475 / \ln 2.7965 = 0.5428$. Here, we notice that the same model is studied on the four-simplex lattice, which belongs to the same universality class as the $b = 2$ 3D SG fractal. In this study [22] the value $\varphi_{32} = 0.5669$ is reported, which appears as an approximate result (and deviates 4% from our exact finding), since in approach applied in [22] some two-SAW configurations are not taken into account (more precisely, the configurations described by function $A_2^{(r)}$, in our notation).

For larger b , that is, for fractals in the range $2 \leq b \leq 40$, we have applied the MCRG method expounded in the previous section. The obtained MCRG values for φ_{32} , together with the pertaining error bars (determined from statistics of measured

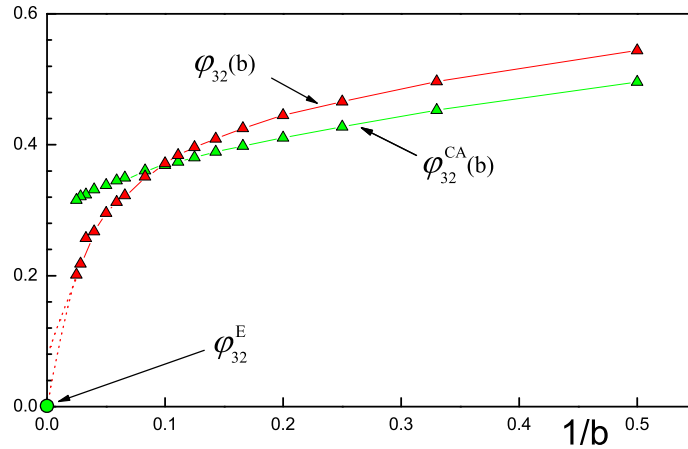


Figure 3. Results obtained in this work for the contact critical exponent φ_{32} for the two-polymer system, when the first polymer is a floating 3D SG chain, while the other is a 2D SG adsorbed chain. The red triangles represent the MCRG values, while green triangles correspond to the CA values calculated from (22). The green circle depicts the tree-dimensional Euclidean value $\varphi_{32}^E \approx 0$. The thin solid lines (red and green) represent a simple interpolation of data, while the red dotted lines show the two possible scenarios for the fractal-to-Euclidean behaviour of φ_{32} , and serve as the guides to the eye. The error bars, for the MCRG data, are not depicted in the figure, since in all cases they lie within of the corresponding symbols (red triangles).

quantities through the Monte Carlo simulations), are given in table 1. The values of φ_{32} for fractals $2 \leq b \leq 30$, have been calculated from averages obtained from 10^6 Monte Carlo simulations performed for each possible two-SAW configuration, while φ_{32} for fractals $b = 35$ and $b = 40$ was obtained performing $5 \cdot 10^5$ Monte Carlo simulations. The time needed to calculate all requisite averages ($\langle N_{A_j} \rangle_{A'_i}^*$, $\langle N_{B_k} \rangle_{A'_i}^*$, $\langle N_{A_j} \rangle_{B'_l}^*$, $\langle N_{B_k} \rangle_{B'_l}^*$) increases exponentially with the scale parameter b , so that for $5 \cdot 10^5$ simulations performed on fractals $b = 10$ and $b = 40$, at the corresponding tricritical fixed points, it was required 10 minutes and 90 hours of the available CPU time, respectively (on a PC with the Intel Pentium 4 processor).

Comparing our MCRG and exact result for $b = 2$ fractal (0.5440 ± 0.0056 versus 0.5428) we can see that the MCRG result deviates 0.22% from the exact RG finding, which is a very well agreement between the two (Monte Carlo and exact) approaches of solving the problem, and thereby provides reliance on accuracy of the MCRG results for larger b . In figure 3 we depict our MCRG findings for the critical exponent φ_{32} , of the 3D SG family of fractals, as a function of $1/b$. We observe that the critical exponent φ_{32} , in the region $2 \leq b \leq 40$, is a monotonically decreasing function of b , which means that the number of polymer contacts (crossings of the SAW paths) decreases with increasing of the fractal dimension of the SG fractals.

In figure 3, we have also presented the numerical values for φ_{32} , that follow from

Table 2. Numerical values for the contact critical exponents φ_{32} , φ_{33} and φ_{22} evaluated from the proposed phenomenological formulae (based on the CA arguments) (22)–(24). The values for ν_3 and ν_2 have been calculated through the MCRG simulations performed in [21] and [24], respectively.

b	ν_3	ν_2	φ_{32}^{CA}	φ_{33}^{CA}	φ_{22}^{CA}
2	0.6742	0.7985	0.4959	0.6516	0.7344
3	0.6543	0.7937	0.4530	0.6287	0.7055
4	0.6414	0.7882	0.4277	0.6140	0.6908
5	0.6315	0.7840	0.4105	0.6050	0.6808
6	0.6239	0.7801	0.3981	0.5984	0.6745
7	0.6169	0.7773	0.3890	0.5953	0.6689
8	0.6130	0.7742	0.3805	0.5887	0.6658
9	0.6087	0.7722	0.3738	0.5855	0.6622
10	0.6048	0.7698	0.3690	0.5833	0.6603
12	0.5987	0.7659	0.3608	0.5792	0.6571
15	0.5933	0.7620	0.3497	0.5711	0.6529
17	0.5899	0.7590	0.3455	0.5683	0.6523
20	0.5869	0.7560	0.3384	0.5621	0.6506
25	0.5817	0.7516	0.3317	0.5577	0.6495
30	0.5795	0.7481	0.3249	0.5502	0.6491
35	0.5759	0.7457	0.3212	0.5490	0.6480
40	0.5755	0.7434	0.3158	0.5416	0.6479

the CA argument predictions adopted for the studied model. Namely, the CA argument claims that a codimension $d - d_{ip}$ of intersection points is a sum of codimensions $d - d_1$ and $d - d_2$ of intersecting objects [16,26]. Here, d is a dimension of embedded space, d_{ip} dimension of intersection points, and, d_1 and d_2 dimensions of intersecting objects. In the studied problem the embedded space is a 3D SG fractal of fractal dimension d_f^{3D} , while the intersecting objects are linear polymers with the fractal dimensions $d_1 = 1/\nu_3$ and $d_2 = 1/\nu_2$, whereupon follows

$$d_{ip} = \left(\frac{1}{\nu_3} + \frac{1}{\nu_2} \right) - d_f^{3D} . \quad (20)$$

On the other hand, the total number of intersection points behaves according to the power law

$$M_{32} \sim \langle R_N \rangle^{d_{ip}} \sim N^{\nu_3 d_{ip}} , \quad (21)$$

where $\langle R_N \rangle \sim N^{\nu_3}$ is the mean end-to-end distance of the longer polymer chain. From the latter scaling form, we find the following phenomenological formula for the contact critical exponent

$$\varphi_{32}^{CA} = \left(1 + \frac{\nu_3}{\nu_2} \right) - \nu_3 d_f^{3D} , \quad (22)$$

whose numerical values, evaluated from the attainable values for ν_3 and ν_2 on SG fractals, are listed in table 2. Comparing the values for φ_{32} predicted by the obtained CA formula with our convincing set of MCRG data (see figure 3), we can perceive that in

the first part of the examined region ($2 \leq b \leq 40$), the CA formula displays satisfactory agreement with the corresponding MCRG values, and, for example, for $b = 10$ fractal the two data (CA and MCRG) have almost identical numerical values. For $b < 10$, the CA formula gives some smaller values for φ_{32} than the MCRG method (at most 9%, for $b = 2$), while for $b > 10$, the CA predicted values get to be larger than the corresponding MCRG findings, and, when b increases, a departure of the two sets of data becomes unambiguous (for $b = 40$, the deviation is 57%). Anyway, from both the MCRG method and the CA formula (22), follow that φ_{32} , in the studied region, is a monotonically decreasing function of b .

Besides of φ_{32} , we may define the critical exponent φ_{33} which describes the number of polymer-polymer contacts, when both polymers are floating chains in the 3D SG fractal container (that is, when both polymers are of the type P_3), and φ_{22} when both polymers are adsorbed by 2D SG surface (both of the type P_2). For these exponents the CA arguments give

$$\varphi_{33}^{CA} = 2 - \nu_3 d_f^{3D}, \quad (23)$$

$$\varphi_{22}^{CA} = 2 - \nu_2 d_f^{2D}. \quad (24)$$

A simple comparison of the data, from table 2, reveals that the following relationship holds

$$\varphi_{32} < \varphi_{33} < \varphi_{22}, \quad (25)$$

for each particular b , in the range $2 \leq b \leq 40$. The first inequality means that the number of polymer contacts increases when both polymers being situated in the bulk of 3D SG fractal, because of growing fractal dimension of a polymer chain when it makes a transition from the 2D SG surface to the bulk of 3D SG fractal ($d_f^{P_3} = 1/\nu_3 > d_f^{P_2} = 1/\nu_2$). On the other hand, in the case when both polymers are adsorbed (situated on 2D SG fractal), the fractal dimension of the embedded space decreases $d_f^{2D} < d_f^{3D}$, and a chance for two polymers to make a contact increases, implying the second inequality in (25).

The relation between φ_{32} and φ_{22} , can be tested on the reliable sets of MCRG values for φ_{32} (calculated in this work) and φ_{22} (calculated previously [18] in the range $2 \leq b \leq 100$). The values for φ_{22} , being always larger than the corresponding CA values proposed by (24), display a monotonic decreasing from $\varphi_{22}(b = 2) = 0.7493$ up to $\varphi_{22}(b = 100) = 0.6735$ [18]. Their comparison with φ_{32} (from table 1) shows that the relation $\varphi_{32} < \varphi_{22}$ is always satisfied. The relations between φ_{33} and the other two contact critical exponents (φ_{32} and φ_{22}) can be numerically proved only for $b = 2$ fractal, where the RG value is known $\varphi_{33}(b = 2) = 0.6635$ [20], and from which the CA value 0.6516 deviates only 1.8%. To complete the inspection of relation (25) and test CA formula (23) for larger b , one needs to calculate φ_{33} values for $b > 2$, which appears to be much complicated task than the calculation of φ_{32} , and may be a topic for a future study.

Finally, we discuss the possible behaviour of the contact critical exponents in the fractal-to-Euclidean crossover region, that is, in the limit $b \rightarrow \infty$ ($d_f^{3D} \rightarrow 3$, $d_f^{2D} \rightarrow 2$). For a SAW situated in Euclidean spaces, the end-to-end distance critical exponent in $d = 2$ takes the exact value $\nu_2^E = 3/4$ [27], that was numerically confirmed [28] for the triangular lattice (to which the 2D SG fractals approach, when $b \rightarrow \infty$), whereas in $d = 3$, at present, the most accurate evaluates are $\nu_3^E = 0.5874 \pm 0.0002$ [29] and $\nu_3^E = 0.58765 \pm 0.00020$ [30]. Consequently, from the formulas (22)–(24), we compute the Euclidean values: $\varphi_{32}^E \approx 0$, $\varphi_{33}^E \approx 1/5$ and $\varphi_{22}^E = 1/2$. In the case of 2D SG fractals (when both polymers are of the type P_2), using the finite-size scaling arguments it was argued [20], that in the limit $b \rightarrow \infty$, the asymptotic behaviour of φ_{22} is described by the relation $\varphi_{22} \simeq 2 - \nu_2 d_f^{2D}$, which coincides with the CA formula (24). Knowing, from the finite-size scaling analysis [31], that ν_2 for very large b goes, from below, to the Euclidean value $3/4$, from the latter asymptotic relation follows that φ_{22} approaches, from above, the Euclidean value $\varphi_{22}^E = 1/2$, when $b \rightarrow \infty$.

As regards the obtained MCRG results for φ_{32} , it is hard to say what happens beyond $b = 40$, and specially, to establish whether the critical exponent φ_{32} , in the limit $b \rightarrow \infty$, goes to the zero Euclidean value, or some non-Euclidean value (see figure 3). To answer this question properly, another method may be needed, for instance, the finite-size scaling approach that has been applied in the case of 2D SG fractals [20, 31]. Here, we can only discuss possible predictions, about the limiting value for φ_{32} , that follow from the corresponding CA formula, for which we need to know the asymptotic behaviour of ν_3 . Unfortunately, up today, the behaviour of ν_3 , in the fractal-to-Euclidean crossover region $b \rightarrow \infty$, exists as an unsolved problem. At this moment, we may say that if $\nu_3 \rightarrow \nu_3^E$ (which means, see data from table 2, that ν_3 is a non-monotonic function of b), then (22) gives $\varphi_{32} \rightarrow \varphi_{32}^E \approx 0$. On the contrary, if ν_3 tends to some non-Euclidean value less than ν_3^E , then φ_{32} will go to some value larger than the Euclidean value φ_{32}^E . The possibility that ν_3 , for $b \rightarrow \infty$, tends to some value larger than ν_3^E should imply a negative value of φ_{32} (and consequently, in this case, we cannot exclude a situation in which the studied transition turns into first order, with increasing b). Similar conclusions may be deduced about the limiting value for the contact critical exponent φ_{33} . Particular, from (23) follows: if $\nu_3 \rightarrow \nu_3^E$ then $\varphi_{33} \rightarrow \varphi_{33}^E \approx 1/5$, or, if ν_3 approaches the non-Euclidean value, then φ_{33} also approaches a non-Euclidean value. From the exposed analysis we may infer that the behaviour of the contact critical exponents, in the fractal-to-Euclidean crossover region, is closely related to the corresponding behaviour of the end-to-end distance critical exponents.

4. Summary

In this paper we have studied the two interacting linear polymer chains, modelled by two mutually crossing SAWs, situated on fractal structures represented by the three-dimensional (3D) Sierpinski gasket (SG) family of fractals. We take on that the first polymer (P_3) is a floating chain in the bulk of 3D SG fractal, while the second polymer

chain (P_2) is adsorbed onto one of the four boundaries of the 3D SG fractal, which appears to be 2D SG fractal. Specifically, we have calculated the contact critical exponent φ_{32} , associated with the number of monomer-monomer contacts between polymers P_3 and P_2 .

By applying the renormalization group (RG) method, we have calculated the exact value of the critical exponent φ_{32} , for the first member $b = 2$ of 3D SG fractal family. The specific accomplishment in the course of this work is the calculation of a long sequence of values of φ_{32} , for $2 \leq b \leq 40$, obtained by applying the Monte Carlo renormalization group (MCRG) method. Our results demonstrate that φ_{32} , for the studied values of b , monotonically decrease with b , and, in analogy with the behaviour of φ_{22} (that governs the number of contacts between two adsorbed polymers) it seems that for $b > 40$ the critical exponent φ_{32} continues decreasing, and in the limit $b \rightarrow \infty$ tends to the Euclidean value $\varphi_{32}^E \approx 0$. Finally, using the codimension additivity (CA) arguments we have proposed the phenomenological formulae for the considered contact critical exponents, and we have tested their predictions on the obtained sets of data. We find that, for fractals labelled by smaller values of b , the CA proposals give satisfactory agreement with existing convincing results.

On the exposed grounds of the presented investigation we may conclude that the set of obtained results of the studied problem has been significantly extended. We have demonstrated that the statistics of two crosslinked polymer chains on the family of 3D SG fractals can be rewardingly studied by the MCRG method. In particular, the MCRG study of the contact critical exponents revealed their interesting behaviour as the functions of fractal scaling parameter b , making a step forward to prescribe the behaviour of SAW critical exponents in the fractal-to-Euclidean crossover region. As a further investigation one may attempt to extend our study for calculating the contact critical exponent φ_{33} , when both polymers are floating chains in the bulk of 3D SG fractal. In addition, to make the studied model more realistic (but more difficult to study), it can be supplemented by additional interactions. For instance, one can introduce the interactions between the bulk floating chain and the sites of adsorbing surface (to promote the adsorbed phase of floating chain), as well as the intra-chain interactions (to promote a collapsing phase of the bulk floating chain), and then, in the space of interaction parameters the phase diagram can be investigated, together with new contact critical exponents at appropriate phase transition fixed points.

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